

The chemical potential of the electron gas on a two dimensional lattice

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Abstract: The chemical potential of the electron gas on a two-dimensional rectangular lattice is determined. An approximate expression for $\exp(-\mu/T)$ is obtained, and its second order approximation is discussed in some detail.

Introduction

Investigations of correlated electron systems of various dimensionality are one of the priorities of contemporary condensed matter physics (for example [1]). The driving force behind the scientific interest in such systems is the fact that they exist in high temperature superconductors and organic conductors. Although the existence of correlated electrons in these materials is regarded as an "established fact", it is far from being completely clear how does one theoretically describe them [2]. The question is if it is possible to use the Fermi liquid model, or the Luttinger liquid model has to be used. For a recent introduction to the Luttinger liquid theory see for example [3].

The aim of the present paper is to calculate the chemical potential of the electron gas on a two dimensional rectangular lattice. Theoretically, this is an interesting problem in itself, and the experimental motivation is amply discussed in the literature (for example [4]). The calculation will be performed within the standard Fermi liquid (FL) model. This presumption could be criticized on the grounds that there are recent results indicating the breakdown of the FL model in cuprate superconductors and heavy-fermion systems (such as [5]). The idea of the present calculation is to contribute to this result, in a different way: by calculating the chemical potential, then separately the electrical conductivity and finally drawing conclusions by comparison with experimental data.

Calculations

The lattice axes are designated by x and y . It can be shown that the number density of a 2D Fermi liquid is given by [6]:

$$n = \frac{\langle N \rangle}{S} = \int \frac{\exp(\beta(\mu - \epsilon))}{1 + \exp(\beta(\mu - \epsilon))} 2 \frac{d^2 p}{(2\pi\hbar)^2} \quad (1)$$

where n denotes the number density and all the other symbols have their usual meanings and $p = \hbar k$. It then follows that $dp = \hbar \frac{\partial k}{\partial \epsilon} d\epsilon$, where ϵ denotes the energy. Accordingly,

$$d^2 p = dp_x dp_y = \hbar^2 \frac{\partial k_x}{\partial \epsilon_x} \frac{\partial k_y}{\partial \epsilon_y} d\epsilon_x d\epsilon_y \quad (2)$$

Assuming that the energy bands along each of the lattice axes have the form $\epsilon = -2t\cos(ks)$, where t denotes the hopping integral and s the lattice constant along the axis, it follows that

$$\frac{\partial k_x}{\partial \epsilon_x} = \frac{1}{2s_x t_x} \frac{d\epsilon_x}{\sqrt{(1 - (\epsilon_x/(2t_x))^2)}} \quad (3)$$

An analogous relation is valid along the y axis. This implies that

$$d^2p = \frac{\hbar^2}{4s_x t_x s_y t_y} \frac{d\epsilon_x d\epsilon_y}{\sqrt{(1 - (\epsilon_x/(2t_x))^2)} \sqrt{(1 - (\epsilon_y/(2t_y))^2)}} \quad (4)$$

Using the expressions for the particle energy along the lattice axes, the exponential factor in eq.(1) can be expressed as

$$\exp(\beta(\mu - \epsilon)) = \exp(\beta(\mu - (\epsilon_x + \epsilon_y))) \quad (5)$$

Inserting eqs.(4) and (5) into eq.(1), after some algebra leads to

$$n = \frac{1}{8\pi^2 s_x t_x s_y t_y} \int \int \frac{d\epsilon_x d\epsilon_y}{1 + \exp(\beta(\epsilon_x + \epsilon_y - \mu))} \frac{1}{\sqrt{(1 - (\epsilon_x/(2t_x))^2)}} \frac{1}{\sqrt{(1 - (\epsilon_y/(2t_y))^2)}} \quad (6)$$

which is the required equation linking various measurable parameters of the electron gas and the lattice with the chemical potential of the electron gas. The limits of integration are $\pm 2t$ along each of the lattice axes, and the problem is how to solve this integral, which can not be done in closed analytical form. Looking at things in a purely mathematical way, the easiest way to solve this integral is to develop the sub-integral function into series. Reasoning in this way, the Fermi distribution function can be re-expressed as follows, under the condition that $\epsilon_x + \epsilon_y < \mu$:

$$\frac{1}{1 + \exp(\beta(\epsilon_x + \epsilon_y - \mu))} = \sum_{l=0}^{l=\infty} (-1)^l \exp(\beta l(\epsilon_x + \epsilon_y - \mu)) \quad (7)$$

Introducing this development into eq.(6), and slightly grouping the terms in it, one gets the following expression:

$$n = \frac{1}{8\pi^2 s_x t_x s_y t_y} \sum_{l=0}^{l=\infty} (-1)^l \int \int \exp(\beta l(\epsilon_x + \epsilon_y - \mu)) \frac{d\epsilon_x d\epsilon_y}{\sqrt{(1 - (\epsilon_x/2t_x)^2)} \sqrt{(1 - (\epsilon_y/2t_y)^2)}} \quad (8)$$

Integrating this expression, within the limits of $\pm 2t$ along both axes, and performing some algebra, leads to the following final result for the filling factor of a Fermi gas on a two dimensional lattice:

$$n = \frac{1}{2s_x s_y} \sum_{l=0}^{\infty} (-1)^l \exp(-\beta \mu l) I_0(2lt_x/\beta) I_0(2lt_y/\beta) \quad (9)$$

where the symbol $I_n(x)$ denotes the modified Bessel function of the first kind of the order n and β is the inverse temperature. The functions $I_n(x)$ are defined by:

$$I_n(x) = \sum_{k=0}^{k=\infty} \frac{(x/2)^{n+2k}}{k! \Gamma(n+k+1)} \quad (10)$$

Discussion

Equation (9) represents the general result of this paper, expressed in its most compact form. The obvious question is the applicability of this result to real physical systems. Limiting the summation in eq(9) to terms with $l \leq 2$ gives

$$n = \frac{1}{2s_x s_y} \left[1 - \exp(-\mu/T) I_0\left(\frac{2t_x}{T}\right) I_0\left(\frac{2t_y}{T}\right) + \exp(-2\mu/T) I_0\left(\frac{4t_x}{T}\right) I_0\left(\frac{4t_y}{T}\right) \right] \quad (11)$$

Solving this equation for $\exp(-\mu/T)$ leads to

$$\exp(-\mu/T) = (I_0(\frac{2t_x}{T})I_0(\frac{2t_y}{T}) \pm \sqrt{I_0^2(\frac{2t_x}{T})I_0^2(\frac{2t_y}{T}) - 4(1 - 2ns_x s_y)I_0(\frac{4t_x}{T})I_0(\frac{4t_y}{T})}) / (2I_0(\frac{4t_x}{T})I_0(\frac{4t_y}{T})) \quad (12)$$

Developing this equation into series up to second order terms in t_x and t_y as small parameters, gives the following expression for $\exp(-\mu/T)$:

$$\exp(-\mu/T) \cong \frac{1}{2}(1 - \sqrt{8ns_x s_y - 3}) + \frac{1}{2}[(t_x/T)^2 + (t_y/T)^2] \left(\frac{16ns_x s_y - 5}{\sqrt{8ns_x s_y - 3}} - 3 \right) + \frac{1}{2} \left(\frac{t_x t_y}{T^2} \right)^2 \left(9 + \frac{16ns_x s_y(9 - 16ns_x s_y) - 17}{(8ns_x s_y - 3)^{3/2}} \right) + . \quad (13)$$

Compare this result with [7] where an expression for the chemical potential of a 1D electron gas has been derived. It follows from eq.(13) that there exists a lower bound on the values of n for which it is applicable. The condition for validity of eq.(13) is $8ns_x s_y - 3 > 0$ which implies $n > \frac{3}{8s_x s_y}$. The implication of this limitation is that eq.(13) can not be used for extremely small values of n . Inspection of this expression shows that it represents the dependence of the chemical potential of a 2D electron gas on various measurable parameters of the system. As the lattice constants along both lattice axes are taken into account, it follows that this equation gives the possibility of analyzing the influence of high external pressure on the chemical potential. This possibility could turn out as being useful in calculations of the pressure dependence of the electrical conductivity of 2D organic conductors.

An interesting problem is the value of n (the filling factor) for which the chemical potential becomes equal to zero. It follows after some algebra that $\mu = 0$ for $n = n_0$, where

$$n_0 = \frac{7T^4 - T^2[1 + 16(t_x^2 + t_y^2)] + 32(t_x^2 + t_y^2)^2}{16s_x s_y(T^2 - 2(t_x^2 + t_y^2))^2 \sqrt{T^4 + 10T^2(t_x^2 + t_y^2) + (t_x^2 + t_y^2)^2}} \quad (14)$$

The outright implication of this result is that the Lieb-Wu theorem [8] is not generally applicable to 2D systems. It can be applied only for certain values of various parameters of the system which enter into eq.(14). It also follows from the last equation that n_0 is a function of the external pressure to which the specimen is subdued.

Conclusions

In this paper we have determined the chemical potential of the electron gas on a 2D rectangular lattice. A general expression linking the filling factor, the chemical potential and various measurable parameters of this system was obtained. Starting from this general expression, an approximate expression for the chemical potential has been obtained. It turns out that this expression is much more complicated than the corresponding expression for a 1D electron gas. This expression can be applied in analyzing real experimental data, and in calculations of the electrical conductivity of Q2D organic metals, which will be done in future work.

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